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Arthur J. Freeman

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Department of Physics & Astronomy
Northwestern University
Evanston IL 60208-3112

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USAF/AFRL
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14. ABSTRACT
To fulfill the great potential of intermetallic alloys for high temperature structural applications, it is necessary to understand the mechanisms controlling their mechanical behavior on the microscopic level, including such key phenomena as dislocation structure and mobility. We focused on the mechanical behavior of homogeneous intermetallics with L12 and B2 structures and on two-phase ./.' alloys. Based on highly-accurate total energy calculations and large-scale Peierls-Nabarro modeling, the relation between electronic structure, phase stability and dislocation structure was investigated in the context of yield stress temperature anomaly (YSA) phenomena, which play a key role in high temperature applications of intermetallic alloys. The superdislocation structure in Ni3Al, Ni3Ge and Fe3Ge was studied and the lack of a yield stress temperature anomaly in Fe3Ge explained. The energetics of the interaction of the {100} edge and screw dislocation in NiAl with different kinds of impurities (Ti, V, Cr, Mn, Zr, Mo, Si, Ge and Ga) was studied and the nature of the "extra" solid solution hardening effect caused by d-element impurities was understood. The origin of the "small" and "large" rhenium effects in Cr-Re alloys was investigated and their mechanisms were proposed.

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PREDICTING ASPECTS OF MECHANICAL BEHAVIOR VIA FUNDAMENTAL ELECTRONIC STRUCTURE CHARACTERISTICS OF HOMOGENEOUS PHASES AND INTRINSIC INTERFACES

AFOSR GRANT No. F49620-01-1-0166

FINAL REPORT

Principal Investigator: Arthur J. Freeman
Dept. of Physics & Astronomy
Northwestern University
Evanston, IL 60208-3112

Abstract

To fulfill the great potential of intermetallic alloys for high temperature structural applications, it is necessary to understand the mechanisms controlling their mechanical behavior on the microscopic level, including such key phenomena as dislocation structure and mobility. We focused on the mechanical behavior of homogeneous intermetallics with $L1_2$ and B2 structures and on two-phase γ/γ' alloys. Based on highly-accurate total energy calculations and large-scale Peierls-Nabarro modeling, the relation between electronic structure, phase stability and dislocation structure was investigated in the context of yield stress temperature anomaly (YSA) phenomena, which play a key role in high temperature applications of intermetallic alloys. The superdislocation structure in Ni_3Al, Ni_3Ge and Fe_3Ge was studied and the lack of a yield stress temperature anomaly in Fe_3Ge explained. The energetics of the interaction of the {100} edge and screw dislocation in NiAl with different kinds of impurities (Ti, V, Cr, Mn, Zr, Mo, Si, Ge and Ga) was studied and the nature of the "extra" solid solution hardening effect caused by d-element impurities was understood. The origin of the "small" and "large" rhenium effects in Cr-Re alloys was investigated and their mechanisms were proposed. The interfacial strength of NiAl/Mo eutectic interfaces was studied and the detrimental effect of the misfit dislocations on it, leading to the interface debonding, was established. The connection between the low temperature yield stress anomaly in Pt_3X alloys with a structural instability rather than with features of the dislocation structure in the $L1_2$ phase was demonstratead. The dislocation structure and character of the yield stress temperature dependence in Ir-based $L1_2$ alloys was predicted. The dislocation structure and energetics in B2 Co-base intermetallics was determined and slip modes operating in these alloys explained. The temperature dependence of the lattice misfit parameter in γ/γ' Ni-, Ir- and Pt-based superalloys were analyzed based on *ab initio* calculations of the thermal expansion.

Executive summary of objectives and accomplishments

The objective of this research is to investigate the microscopic mechanisms governing the deformation and fracture behavior of ordered intermetallic aerospace alloys in order to contribute to the development of a fundamental basis for computer-aided alloys design. The most important and challenging component of our research is to bridge the gap between a microscopic quantum-mechanical description of the chemical bonding and the mesoscopic phenomena which govern the mechanical response of intermetallics. The emphasis on the computational/simulation approach focuses on understanding "real" materials, which have an abundance of "defects" including impurities, dislocations or other faults, second phase precipitates, etc. - all of which are governed on the microscopic level by the electronic structure.

1. Superdislocation core structure in $L1_2$ Ni_3Al, Ni_3Ge and Fe_3Ge via an ab initio GSF-Peierls-Nabarro approach.

It is now well established that yield stress anomaly (YSA) is the intrinsic property of most $L1_2$ intermetallics originating in the structure and properties of superdislocations. The quasi-binary system Ni_3Ge-Fe_3Ge is an example of a gradual transition from anomalous to normal behavior as Fe is substituted for Ni. This is an attractive feature for studying mechanisms of the temperature anomaly - a property widely used in structural alloys and driven by features of the dislocation core structure.

Superdislocation core structure in $L1_2$ Ni_3Al, Ni_3Ge and Fe_3Ge was studied using an *ab initio* GSF-Peierls-Nabarro approach. Stacking fault energies, theoretical values of the separation between dislocation superpartials and Shockley partials, and dislocation "splitting paths" were calculated. Two types of superdislocations are predicted as possible in Ni_3Al and only the type I superdislocation in Ni_3Ge. The Fe_3Ge presents the opposite case; type I superdislocations do not exist and only type II may be realized in a stable configuration. The disappearance of type I superdislocations, due to unstable APB energy, is found to be the main reason for the lack of a yield stress temperature anomaly in Fe_3Ge.

2. Energetics and mechanism of impurity-dislocation interactions in NiAl.

The improvement of the strength of materials due to doping by ternary additions has become a traditional alloy design approach. According to the prevailing point of view, the size misfit between the impurity and host atoms appears to make the main contribution in impurity-dislocation interaction and solid solution hardening (SSH) in a majority of alloys. In NiAl and Ni_3Al, however, SSH differs significantly for elements with similar atomic radii: it is very high for early 3d, 4d and 5d elements ("extra" SSH), but low for B-subgroup elements.

The energetics of the interaction of the $\langle 100 \rangle \{010\}$ edge dislocation in NiAl with different kinds of impurities (Ti, V, Cr, Mn, Zr, Mo, Si, Ge and Ga) was studied using the *ab initio* real-space tight-binding LMTO-recursion method. A strong interaction with 3d and 4d element impurities is found (dislocation locking). The nature of the locking is due to the strong hybridization and preferred bonding between the electronic states of the impurity atom and the localized electronic states forming in the center of the dislocation core. The

electronic contribution to the interaction of B-subgroup elements Si, Ge and Ga with the ⟨100⟩{010} edge dislocation in NiAl is found to be small, and the impurity-dislocation interaction is controlled by the elastic mechanism. These findings explain the "extra" solid solution hardening effect caused by d-element impurities and emphasize the importance of the electronic mechanism.

3. Interaction of transition metal impurities with screw dislocations in NiAl.

It is traditionally believed that the solid solution hardening (SSH) effect of impurities is caused by the impurity-dislocation interaction due to size misfit between the impurity and host atoms (parelastic mechanism). For screw dislocations, which cause much smaller dilatations to the crystal lattice than edge dislocations, parelastic impurity-dislocation interactions are expected to be very small, and it is traditionally believed that screw disocations do not contribute to SSH.

The energetics of interactions of the ⟨100⟩{010} screw dislocation with early 3d element impurities (Ti, V, Cr, Mn) in NiAl was investigated, and strond attractive interaction (dislocation locking) was found. Thus, the universality of the electronic mechanism of impurity-dislocation interactions without regard to the dislocation orientation (edge or screw) is demonstrated, in contrast to parelastic mechanisms (size and modulus misfit).

4. Electronic structure, Fermi surface and mechanical behavior of bcc Cr-Re alloys. Mechanism of the "rhenium effect".

Alloys based on the VI-A group refractory bcc metals (Cr, Mo, W) are attractive materials for high-temperature applications. Among them, chromium alloys have advantages due to low density, high creep and oxidation resistance. So far, the practical potential of these alloys has not been realized because of their room-temperature brittleness. A significant improvement in the mechanical properties (both strength and plasticity) of these metals can be achieved by alloying with rhenium at 5-6 at.% ("small" rhenium effect) or at concentration close to the solubility limit – the so-called ("large rhenium effect). Significant efforts have been made to explain the "large" rhenium effect, while the nature of the "small" rhenium effect is still unclear.

The electronic structure, chemical bonding and ground state characteristics of Cr-Re alloys in a wide range of Re concentration were investigated using the first-principles full-potential linear muffin-tin orbital (FLMTO) method. It was demonstrated that particles of the Cr_3Re close-packed phase with A15 structure can be formed stabilized by carbon and act as scavengers of light impurities, thus improving the ductility of Cr and contributing to the "large rhenium effect".

The Fermi surface topology of Cr-Re alloys at different concentrations was investigated. Two electronic topological transitions (ETT) were found at 6 at.% Re and at 18 at.% Re. The "small rhenium effect" is found to be closely connected with the softening of Cr–Cr nearest-neighbor bonds due to the ETTs.

5. Interface strength of the NiAl/Mo eutectic composite. Adhesion and misfit dislocation energies.

The fracture toughness of brittle intermetallics can be improved by the reinforcement with ductile phases. There is a considerable promise in NiAl/X eutectic composites with refractory metal (X = W, Mo, Cr, V) reinforcement. The potential of this composite was not completely realized because of the low ductility of the reinforcing bcc metal phase and weak interface leading to crack interface debonding. For further progress, it is important to improve our understanding of the physical factors controlling the interfacial strength and plasticity of the refractory phase.

The ideal interfacial work of adhesion for the NiAl/Mo interface was calculated using the FLMTO method. The interface is found to be Ni-terminated, and the interface adhesion energy is intermediate between bulk NiAl and Mo, indicating that the ideal interface is not intrinsically weak. The effect of misfit dislocations on the interfacial energy was studied using the modified *ab initio* GSF-Peierls-Nabarro approach. It was found that the misfit dislocation energy significantly reduces the adhesion of the interface – by approximately 30%. As a result, the interface strength becomes lower than the strength of bulk NiAl, and the formation of misfit dislocations is the main reason for interface debonding in NiAl/Mo eutectics.

6. Negative yield stress temperature anomaly, structural stability, and dislocation structure of Pt_3Al.

It is now well established that the anomalous temperature dependent yield stress (YS), is an intrinsic property of ordered $L1_2$ alloys originating in the structure and properties of superdislocations. The Pt_3X (X = Al, Ga, Ge) series of intermetallics is known to have a strong negative temperature dependence of the YS in contrast with other $L1_2$ type compounds like Ni_3Al. It is well established experimentally that in Pt_3X, primary superdislocation cube glide takes place which leads to a normal YS dependence (so-called negative or low temperature anomaly (LTA)). The question about the mechanism of the LTA behavior in Pt_3Al is still open.

The electronic structure, total energy and chemical bonding of stoichiometric Pt_3Al and aluminum-doped $Pt_{72}Al_{28}$ and $Pt_{69}Al_{31}$ alloys in the $L1_2$, $D0_c$, and $D0_c'$ structures were investigated by the all-electron full-potential linearized augmented plane wave (FLAPW) method. The $D0_c'$ structure, rather than traditionally assumed $L1_2$ structure, was found to be energetically preferable for Pt_3Al. The deviation from stoichiometry toward Al leads to stabilization of the $L1_2$ phase at 6 at. % Al doping.

The dislocation structure of the $L1_2$ and $D0_c'$ phases was calculated based on the combined *ab initio*-Peierls-Nabarro approach. It was found that the small atomic displacements that accompany the $L1_2 \rightarrow D0_c'$ transition lead to drastic changes in dislocation energetics and in the mechanical behavior of Pt_3Al. The origins of the LTA were revealed and the main peculiarities of the mechanical behavior of Pt_3Al, such as the large anisotropy of the shear resistance and sensitivity to deviations from stoichiometry, were explained.

7. Dislocation structure and mechanical behavior of Ir-based $L1_2$ alloys.

Modern two-phase γ/γ' nickel-based superalloys find a wide range of high temperature applications. A new approach for the development of high-temperature superalloys is based on using platinum group metals with higher melting temperatures and superior environmental properties. In particular, binary Ir-Nb alloys are the strongest high-temperature materials developed to date. Unfortunately, there is no reliable information about dislocation structure and mobility in Ir_3X alloys (X = Nb, Ti, Zr, Ta), and the mechanisms driving the YS temperature dependence in Ir_3X are unclear.

The dislocation properties of Ir_3X alloys were investigated using the *ab initio*-Peierls-Nabarro approach. The superdislocations with a type II core structure are strongly preferable energetically in Ir_3Ta and Ir_3Nb, whereas type I superdislocations are predicted in Ir_3Ti and Ir_3Zr. Because type I superdislocations are usually considered as responsible for the YSA, our results predict that a positive yield stress temperature dependence should be expected in Ir_3Zr and Ir_3Ti, and a negative YS behavior in Ir_3Nb and Ir_3Ta. The dislocation structure and the resulting features of the mechanical behavior in Ir-based alloys are found to be closely connected with the phase instability related to the $L1_2 \rightarrow D0_{19}$ transformation.

8. Yield stress temperature anomaly in B2 CoX (X = Ti, Zr, Hf); features of the ⟨100⟩ dislocation structure.

Cobalt-based B2 intermetallics (CoTi, CoZr, CoHf) are unique alloys that exhibit a positive yield stress dependence on temperature, which is usually associated with thermally activated locking of ⟨111⟩ superdislocations, yet demonstrate only ⟨100⟩ slip. The reasons for such an unusual behavior are not yet clear.

Shear properties of CoTi were determined on the basis of FLMTO total energy calculations, and structure and properties of dislocations for several slip planes were studied. GSF energies for {100} and {110} planes in CoTi were found to be significantly smaller compared to NiAl, and the lowest shear resistance corresponds to the {110} slip plane. The low GSF energy in CoTi for {110} shear results in a wide dislocation core with a width that is three times larger than in NiAl. A strong preference for ⟨100⟩{110} slip was found, in agreement with experiment. The distinctive features of the dislocation structure in CoTi originate from both the low value of the C_{44} elastic constant and the small GSF energy of ⟨100⟩{110} shear and are closely connected with the lattice instability of B2 CoTi with respect to the B19' structure.

9. Temperature dependence of the lattice misfit; ab initio calculations for γ/γ' superalloys.

The magnitude of the lattice misfit between the γ and γ' phases, is one of the key parameters which determines the microstructure formation, stability and mechanical behavior of modern high-temperature superalloys. At present, it is still unclear whether the misfit changes at high temperatures are caused by either compositional changes of the phases or by differences in the thermal expansion coefficients.

The role of thermal expansion in the temperature dependence of the lattice misfit in the

Ni/Ni_3Al, Ir/Ir_3Nb, and Pt/Pt_3Al γ/γ' superalloys was explored on the basis of *ab initio* calculations of electron and phonon spectra. It was found that the electron contributions to the thermal expansion of γ and γ' phases dominate the misfit dependence even at high temperatures because of an important cancellation of the phonon contributions. The thermal expansion contribution to the variation of the lattice misfit was found to be prevailing for Ir- and Pt-based superalloys, while for Ni/Ni_3Al a redistribution of the alloying component should also be taken into account.

Personnel Supported

Oleg Y. Kontsevoi	Research Associate, Northwestern University, Evanston, IL
Yuri N. Gornostyrev	Visiting Research Scientist from Institute of Metal Physics, Ekaterinburg, Russia
Nadezhda I. Medvedeva	Visiting Research Scientist from Institute of Solid State Chemistry, Ekaterinburg, Russia
Oleg N. Mryasov	Research Scientist, Sandia National Laboratory, Livermore, CA
Konstantin Y. Khromov	Visiting Research Scientist from Russian Science Center "Kurchatov Institute", Moscow, Russia
Andrey F. Maksyutov	Visiting Predoctoral Fellow from Russian Science Center "Kurchatov Institute", Moscow, Russia

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9. "Negative yield stress temperature anomaly and structural instability of Pt_3Al", Yu.N. Gornostyrev, O.Yu. Kontsevoi, A.F. Maksyutov, A.J. Freeman, M.I. Katsnelson, A.V. Trefilov, and A.I. Lichtenshtein, Physical Review B, Vol. 70, No.1, Art. No. 014102 (2004).
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12. "Dislocation structure, phase stability and yield stress behavior of $L1_2$ intermetallics: Ir_3X (X = Ti, Zr, Hf, V, Nb, Ta)", O.Yu. Kontsevoi, Yu.N. Gornostyrev, A.F. Maksyutov, K.Yu. Khromov, and A.J. Freeman, Metallurgical and Materials Transactions A (accepted).
13. "Strong "chemical interactions" of transition metal impurities with edge and screw dislocations in NiAl: electronic mechanism of", O.Yu. Kontsevoi, Yu.N. Gornostyrev, and A.J. Freeman, Physical Review B (submitted).
14. "Electronic and lattice contributions to the temperature dependence of misfit parameter in two-phase refractory superalloys", Yu.N. Gornostyrev, O.Yu. Kontsevoi, K.Yu. Khromov, A.F. Maksyutov, A.J. Freeman, M.I. Katsnelson, and A.V. Trefilov, Physical Review B (submitted).
15. "New Features of Dislocation Structures Originating in Lattice Discreteness", O.N. Mryasov, Yu.N. Gornostyrev, and A.J. Freeman, Physical Review B (submitted), cond-mat/0006257.

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1. "Electronic mechanism of impurity-dislocation interactions in intermetallics", O.Yu. Kontsevoi, A.J. Freeman, and Yu.N. Gornostyrev, American Physical Society Meeting, March 12-16, 2001, Seattle, WA.
2. "First-principles investigation of the rhenium effect in Cr-based alloys", N.I. Medvedeva, Yu.N. Gornostyrev, and A.J. Freeman, American Physical Society Meeting, March 12-16, 2001, Seattle, WA.
3. "Ab initio generalized stacking fault energetics and structure of dislocations in $L1_2$ intermetallics", O.N. Mryasov, M. van Schilfgaarde, Yu.N. Gornostyrev, and A.J.

Freeman, American Physical Society Meeting, March 12-16, 2001, Seattle, WA.

4. "Bonding, energetics and mechanical properties of intermetallics", A. J. Freeman, Yu. N. Gornostyrev, O. N. Mryasov, O. Yu. Kontsevoi, and N.I. Medvedeva, AFOSR Joint Metallic and Ceramic Materials Programs Review Meeting, August 19-21, 2001, Snowbird, UT.
5. "Interaction of the <100> screw dislocation in NiAl with transition metal impurities: electronic mechanism", O.Yu. Kontsevoi, Yu.N. Gornostyrev, and A.J. Freeman, American Physical Society Meeting, March 18-22, 2002, Indianapolis, IN.
6. "Magnetic, structural and mechanical properties of Cr and Cr-Re alloys", N.I. Medvedeva, Yu.N. Gornostyrev, and A.J. Freeman, American Physical Society Meeting, March 18-22, 2002, Indianapolis, IN.
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9. "Ab initio total-energy calculations of cleavage decohesion and shear processes and dislocation structure in CoTi", O.Yu. Kontsevoi, Yu.N. Gornostyrev, and A.J. Freeman, American Physical Society Meeting, March 3-7, 2003, Austin, TX.
10. "Negative yield stress temperature anomaly and structural stability of Pt_3Al", Yu.N. Gornostyrev, A.F. Maksyutov, O.Yu. Kontsevoi, A.J. Freeman, M.I. Katsnelson, and A.V. Trefilov, American Physical Society Meeting, March 3-7, 2003, Austin, TX.
11. "Fundamental electronic structure characteristic and mechanical behavior of intermetallics", AFOSR Contractors Meeting in Metallic Materials, August 4-5, 2003, Boulder, CO.